IN THE CLAIMS:

The text of all pending claims, (including withdrawn claims) is set forth below. Cancelled and not entered claims are indicated with claim number and status only. The claims as listed below show added text with <u>underlining</u> and deleted text with ~~strikethrough~~. When strikethrough cannot easily be perceived, or when five or fewer characters are deleted, [[double brackets]] are used to show the deletion. The status of each claim is indicated with one of (original), (currently amended), (cancelled), (withdrawn), (new), (previously presented), or (not entered). Please AMEND claims 5-11 and 21, and ADD new claims 25-27 in accordance with the following:

1-4.   (cancelled)

5.   (currently amended) A method of analyzing three-dimensional structures <u>of a predetermined amino acid sequence probe and a protein molecule target, wherein the predetermined amino acid sequence probe includes</u> ~~including~~ a first structure expressed by three-dimensional coordinates of elements belonging to a first point set and <u>the protein molecule target includes</u> a second structure expressed by three-dimensional coordinates of elements belonging to a second point set<u>, to determine a degree of similarity between the three dimensional structure of the predetermined amino acid sequence probe represented by the three-dimensional coordinates of the elements belonging to the first point set and the three-dimensional structure of the protein molecule target represented by the three-dimensional coordinates of elements belonging to the second point set</u>, comprising:

~~a)~~ generating, by a superposition calculating unit, a combination of correspondence satisfying a condition between the elements belonging to the first point set and the elements belonging to the second point set from among all candidates for the combination of correspondence, <u>wherein the condition includes generating a desired combination based on a predetermined minimized geometric distance between the first and second point sets, setting a predetermined threshold value and pruning a retrieval path if an attribute value of a candidate is greater than the predetermined threshold value, and determining that a point is a candidate if an attribute of an element of the first point set includes a type of an atom, an atomic group, and a molecule, a hydrophilic property, a hydrophobic property, or a positive or negative charge that coincides with an attribute of an element of the first point set,</u>~~wherein the condition includes generating an optimum combination in view of at least one of a geometric relationship between the first and second point sets, a threshold value condition in relating the elements of the first and second point sets,~~ and refining the elements of the first and second point sets based on ~~at~~

2

~~least one of~~ an attribute of the elements of the first and second point sets;

~~b)~~ calculating, by the superposition calculating unit, a root mean square distance between the elements belonging to the first point set relating to the elements belonging to the second point set in the <u>generated</u> combination of correspondence ~~generated in the generating~~; ~~and~~

~~c)~~ <u>determining, by the superposition calculating unit, based on the generated combination of correspondence and minimizing root mean square distance values, similar portions of the three dimensional structure of the predetermined amino acid sequence probe represented by the three-dimensional coordinates of the elements belonging to the first point set and the three-dimensional structure of the protein molecule target represented by the three-dimensional coordinates of elements belonging to the second point set; and</u>

displaying, by a graphic display unit, the three-dimensional structures of the ~~first structure~~ <u>predetermined amino acid sequence</u> and the <u>protein molecule</u> ~~second structure~~ in an overlapped manner based on the ~~calculating~~ <u>generated combination of correspondence and minimized root mean square distance values</u>,

~~wherein the first and second three-dimensional structures are at least one of a protein molecule, and~~

wherein the first and second point sets<u>, respectively,</u> are sequence listings defining <u>the predetermined amino acid sequence probe and the protein molecule target, respectively.</u> ~~the first and second three-dimensional structures.~~

6.   (currently amended) ~~A~~ <u>The</u> method of claim 5, wherein the condition includes order relation of the elements in the first and the second point sets that are ordered.

7.   (currently amended) ~~A~~ <u>The</u> method of claim 5, wherein the condition includes proximity in a geometric relationship among a plurality of elements close to each other.

8.   (currently amended) ~~A~~ <u>The</u> method of claim 6 wherein the condition includes proximity in a geometric relationship among a plurality of elements close to each other.

9.   (currently amended) ~~A~~ <u>The</u> method of claim 5, wherein the condition includes a condition such that a candidate for the combination of correspondence satisfies a threshold value condition.

10.   (currently amended) A The method of claim 6, wherein the condition includes a condition such that a candidate for the combination of correspondence satisfies a threshold value condition.

11.   (currently amended) A The method of claim 5, wherein the condition includes a condition such that an attribute value of each of the elements belonging to the first point set coincides with an attribute value of the corresponding element belonging to the second point set in a candidate for the combination of correspondence.

12-20. (cancelled)

21.   (currently amended) An apparatus for analyzing three-dimensional structures of a predetermined amino acid sequence probe and a protein molecule target, wherein the predetermined amino acid sequence includes including a first structure expressed by three-dimensional coordinates of elements belonging to a first point set and the protein molecule target includes a second structure expressed by three-dimensional coordinates of elements belonging to a second point set, to determine a degree of similarity between the three dimensional structure of the predetermined amino acid sequence probe represented by the three-dimensional coordinates of the elements belonging to the first point set and the three-dimensional structure of the protein molecule target represented by the three-dimensional coordinates of elements belonging to the second point set, comprising:

a superposition calculating unit generating a combination of correspondence satisfying a condition between the elements belonging to the first point set and the elements belonging to the second point set from among all candidates for the combination of correspondence, and calculating a root mean square distance between the elements belonging to the first point set relating to the elements belonging to the second point set in the combination of correspondence generated, wherein the condition includes generating a desired combination based on a predetermined minimized geometric distance between the first and second point sets, setting a predetermined threshold value and pruning a retrieval path if an attribute value of a candidate is greater than the predetermined threshold value, and determining that a point is a candidate if an attribute of an element of the first point set includes a type of an atom, an atomic group, and a molecule, a hydrophilic property, a hydrophobic property, or a positive or negative charge that coincides with an attribute of an element of the first point set, wherein the condition includes generating an optimum combination in view of at least one of a geometric relationship between

4

~~the first and second point sets, a threshold value condition in relating the elements of the first~~ ~~and second point sets,~~ and refining the elements of the first and second point sets based on ~~at~~ ~~least one of~~ an attribute of the elements of the first and second point sets; and determining, based on the generated combination of correspondence and minimizing root mean square distance values, similar portions of the three dimensional structure of the predetermined molecular structure probe represented by the three-dimensional coordinates of the elements belonging to the first point set and the three-dimensional structure of the molecular structure target represented by the three-dimensional coordinates of elements belonging to the second point set; and

a graphic display unit displaying the three-dimensional structures of the first structure and the second structure in an overlapped manner based on the <u>calculated combination of</u> <u>correspondence</u> and the minimized root mean square distance values~~calculating~~,

~~wherein the first and second three-dimensional structures are at least one of a protein~~ ~~molecule, and~~

wherein the first and second point sets<u>, respectively,</u> are sequence listings defining the <u>predetermined amino acid sequence target and the protein molecule target, respectively,</u> ~~first~~ ~~and second three-dimensional structures.~~

22-23. (cancelled)

24.   (previously presented) The method of claim 6, wherein the condition includes a condition such that an attribute value of each of the elements belonging to the first point set coincides with an attribute value of the corresponding element belonging to the second point set in a candidate for combination of correspondence.

25.   (new) A method of analyzing three-dimensional structures of a predetermined molecular structure probe and a molecular structure target, wherein the predetermined molecular structure probe includes a first structure expressed by three-dimensional coordinates of elements belonging to a first point set and the molecular structure target includes a second structure expressed by three-dimensional coordinates of elements belonging to a second point set, to determine a degree of similarity between the three dimensional structure of the predetermined molecular structure probe represented by the three-dimensional coordinates of the elements belonging to the first point set and the three-dimensional structure of the molecular structure target represented by the three-dimensional coordinates of elements belonging to the

second point set, comprising:

generating, by a superposition calculating unit, a combination of correspondence satisfying a condition between the elements belonging to the first point set and the elements belonging to the second point set from among all candidates for the combination of correspondence, wherein the condition includes generating a desired combination based on a predetermined minimized geometric distance between the first and second point sets, setting a predetermined threshold value and pruning a retrieval path if an attribute value of a candidate is greater than the predetermined threshold value, and determining that a point is a candidate if an attribute of an element of the first point set includes a type of an atom, an atomic group, and a molecule, a hydrophilic property, a hydrophobic property, or a positive or negative charge that coincides with an attribute of an element of the first point set, and refining the elements of the first and second point sets based on an attribute of the elements of the first and second point sets; calculating, by the superposition calculating unit, a root mean square distance between the elements belonging to the first point set relating to the elements belonging to the second point set in the generated combination of correspondence;

determining, by the superposition calculating unit, based on the generated combination of correspondence and minimizing root mean square distance values, similar portions of the three dimensional structure of the predetermined molecular structure probe represented by the three-dimensional coordinates of the elements belonging to the first point set and the three-dimensional structure of the molecular structure target represented by the three-dimensional coordinates of elements belonging to the second point set; and

displaying, by a graphic display unit, the three-dimensional structures of the predetermined molecular structure probe and the molecular structure target in an overlapped manner based on the generated combination of correspondence and minimized root mean square distance values,

wherein the first and second point sets, respectively, are sequence listings defining the predetermined molecular structure probe and the molecular structure target, respectively.

26. (new) A computer-readable medium containing computer-readable instructions to analyze three-dimensional structures of a predetermined molecular structure probe and a molecular structure target, wherein the predetermined molecular structure probe includes a first structure expressed by three-dimensional coordinates of elements belonging to a first point set and the molecular structure target includes a second structure expressed by three-dimensional coordinates of elements belonging to a second point set, to determine a degree of similarity

between the three dimensional structure of the predetermined molecular structure probe represented by the three-dimensional coordinates of the elements belonging to the first point set and the three-dimensional structure of the molecular structure target represented by the three-dimensional coordinates of elements belonging to the second point set, the computer-readable instructions comprising:

generating a combination of correspondence satisfying a condition between the elements belonging to the first point set and the elements belonging to the second point set from among all candidates for the combination of correspondence, wherein the condition includes generating a desired combination based on a predetermined minimized geometric distance between the first and second point sets, setting a predetermined threshold value and pruning a retrieval path if an attribute value of a candidate is greater than the predetermined threshold value, and determining that a point is a candidate if an attribute of an element of the first point set includes a type of an atom, an atomic group, and a molecule, a hydrophilic property, a hydrophobic property, or a positive or negative charge that coincides with an attribute of an element of the first point set, and refining the elements of the first and second point sets based on an attribute of the elements of the first and second point sets; calculating, by the superposition calculating unit, a root mean square distance between the elements belonging to the first point set relating to the elements belonging to the second point set in the generated combination of correspondence;

determining, based on the generated combination of correspondence and minimizing root mean square distance values, similar portions of the three dimensional structure of the predetermined molecular structure probe represented by the three-dimensional coordinates of the elements belonging to the first point set and the three-dimensional structure of the molecular structure target represented by the three-dimensional coordinates of elements belonging to the second point set; and

causing to be displayed, on a display, the three-dimensional structures of the predetermined molecular structure probe and the molecular structure target in an overlapped manner based on the generated combination of correspondence and minimized root mean square distance values,

wherein the first and second point sets, respectively, are sequence listings defining the predetermined molecular structure probe and the molecular structure target, respectively.

27. (new) An apparatus for analyzing three-dimensional structures of a predetermined molecular structure probe and a molecular structure target, wherein the predetermined

molecular structure probe includes a first structure expressed by three-dimensional coordinates of elements belonging to a first point set and the molecular structure target includes a second structure expressed by three-dimensional coordinates of elements belonging to a second point set, to determine a degree of similarity between the three dimensional structure of the predetermined molecular structure probe represented by the three-dimensional coordinates of the elements belonging to the first point set and the three-dimensional structure of the molecular structure target represented by the three-dimensional coordinates of elements belonging to the second point set, comprising:

a database having data having stored therein that includes a plurality of three-dimensional molecular structures of substances representing a plurality of predetermined molecular structure probes, each having a first structure expressed by three-dimensional coordinates of elements belonging to a first point set;

a data input unit that reads the data and an input command from a user selecting a molecular structure target that includes the second structure expressed by three-dimensional coordinates of elements belonging to the second point set;

a superposition calculation unit that generates a combination of correspondence satisfying a condition between the elements belonging to the first point set and the elements belonging to the second point set from among all candidates for the combination of correspondence, wherein the condition includes generating a desired combination based on a predetermined minimized geometric distance between the first and second point sets, setting a predetermined threshold value and pruning a retrieval path if an attribute value of a candidate is greater than the predetermined threshold value, and determining that a point is a candidate if an attribute of an element of the first point set includes a type of an atom, an atomic group, and a molecule, a hydrophilic property, a hydrophobic property, or a positive or negative charge that coincides with an attribute of an element of the first point set, determines a degree of similarity between the three dimensional structure of the predetermined molecular structure probe represented by the three-dimensional coordinates of the elements belonging to the first point set and the three-dimensional structure of the molecular structure target represented by the three-dimensional coordinates of elements belonging to the second point set, and superposes a three-dimensional molecular structure of a predetermined molecular structure probe read from the database with a three-dimensional molecular structure target in accordance with the desired combination and having minimized root mean square distance values; and

a graphic display unit that displays the three-dimensional structures of the predetermined molecular structure probe and the molecular structure target in an overlapped manner based on

the calculations of the superposition calculation unit.